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Symmetry-Protected Topological Orders in Interacting Bosonic Systems

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Symmetry-protected topological (SPT) phases are bulk-gapped quantum phases with symmetries, which have gapless or degenerate boundary states as long as the symmetries are not broken. The SPT phases in free fermion systems, such as topological insulators, can be classified; however, it is not known what SPT phases exist in general interacting systems. We present a systematic way to construct SPT phases in interacting bosonic systems. Just as group theory allows us to construct 230 crystal structures in three-dimensional space, we use group cohomology theory to systematically construct different interacting bosonic SPT phases in any dimension and with any symmetry, leading to the discovery of bosonic topological insulators and superconductors.

For many years, the defining characteristic of a phase of matter was thought to be its symmetry, with different phases necessarily having different symmetries (1). However, through the study of high-temperature superconductors and the fractional quantum Hall (FQH) effect, it was discovered that there can be distinct quantum phases—topologically ordered phases—that cannot be distinguished by symmetry (2). A deep connection between quantum phases and quantum entanglement (3–5) indicates that topological orders are characterized by patterns of long-range entanglement (5). Recently, it was discovered that even short-range entangled states with the same symmetry can belong to different phases. These symmetric short-range entangled states are said to contain a new kind of order called symmetry-protected topological (SPT) order, (6) which is characterized by symmetry-protected gapless or degenerate edge states despite the bulk gap. Just like symmetry-breaking orders are described by group theory, we show here that SPT orders are described by group cohomology theory. This discovery expands our original understanding of possible phases in many-body systems.

A central issue is to understand what SPT phases exist. The first system known to have SPT order was the spin-1 chain with antiferromagnetic Heisenberg interactions (the so-called Haldane chains) (7, 8). This model has been generalized, leading to a complete classification of SPT orders in one-dimensional (1D) bosonic/fermionic systems (9–12). Topological insulators (13–17) with gapless edge modes protected by time-reversal symmetry and particle-number

conservation provided the first example of an SPT order in higher dimensions. The noninteracting nature of fermions in these systems allows a classification of this kind of SPT order (18, 19), whereas no SPT order exists in noninteracting bosonic systems.

However, understanding SPT orders in noninteracting systems is not sufficient, because particles in real materials do interact. In this paper, we present a systematic construction of SPT phases for interacting bosonic systems in any dimension and with any symmetry. Our construction leads to the discovery of many SPT phases in 2 and higher dimensions (see Table 1). For simplicity, we are going to first present in detail the case of the 1D Haldane chain and demonstrate the emergence of its SPT order using the group cohomology theory for time reversal symmetry. The group cohomology approach allows us to generalize the construction to higher dimensions and to all other symmetries.

The fixed-point ground-state wave function of the Haldane chain (6) takes a simple dimer form (Fig. 1), where each site contains two spin 1/2's connected into singlet pairs $|\uparrow_i^r \downarrow_{i+1}^l\rangle - |\downarrow_i^r \uparrow_{i+1}^l\rangle$ between neighboring sites (20). Time-reversal

symmetry acts as $M(T) = i\sigma_y K$ on each spin 1/2, where K is complex conjugation and σ_y is the y component of the spin operator. The wave function is invariant under the symmetry action. For each spin 1/2, $M(T)^2 = -I$, whereas on each site with two spins, $[M(T) \otimes M(T)]^2 = I$. So the states on each site form a representation of Z_2^T , the symmetry group generated by time reversal symmetry.

The wave function on a closed chain is the gapped ground state of the Hamiltonian $H = \sum_i \sigma_i^r \cdot \sigma_{i+1}^l$, with antiferromagnetic Heisenberg interactions between each pair of spin 1/2's on neighboring sites where σ_i^l and σ_i^r are spin operators for the left and right spin 1/2 on each site, respectively. The Hamiltonian is invariant under time-reversal symmetry; the ground state does not break any symmetry of the system, yet the system is far from a trivial phase, which becomes evident when we put the system on an open chain. When the chain is open, the dangling spin 1/2 at each end forms a nontrivial projective representation of Z_2^T with $M(T)^2 = -I$, which does not allow a 1D representation (21). Therefore, the degeneracy of the edge state is robust under any perturbation as long as time-reversal symmetry is preserved.

The ground-state structure giving rise to SPT order in the Haldane chain can be generalized to an arbitrary symmetry group after we relabel the spin states with group elements and express symmetry actions using group cocycles. The time-reversal symmetry group contains two elements: $Z_2^T = \{E, T\}$ with $T \circ T = E$. For the left spin 1/2 on each site, label $|\uparrow\rangle/|\downarrow\rangle$ as $|E\rangle/|T\rangle$, and for the right one, label $|\uparrow\rangle/|\downarrow\rangle$ as $|E\rangle/|-T\rangle$. The total wave function becomes

$$|\Phi\rangle = \prod_i (|T_i^r T_{i+1}^l\rangle + |E_i^r E_{i+1}^l\rangle) = \prod_i \sum_{g_i} |g_i^r = g_i, g_{i+1}^l = g_i\rangle \quad (1)$$

where $g_i \in Z_2^T$. Time-reversal symmetry then acts on the right/left spins on each site as $M(T)|E\rangle = -|T\rangle$ and $M(T)|T\rangle = |E\rangle$, which takes the form

Table 1. SPT phases in d spatial dimensions protected by some simple symmetries (represented by the symmetry groups). Z_1 means that our construction only gives rise to the trivial phase. Z_n^m means that the constructed nontrivial SPT phases plus the trivial phase are labeled by m elements in Z_n . Z means that the constructed nontrivial SPT phases are labeled by nonzero integers, whereas the trivial one is labeled by 0. Z_2^T represents time-reversal symmetry, $U(1)$ represents boson number—conservation symmetry, $SO(3)$ represents rotation symmetry, Z_n represents cyclic symmetry of order n , and D_2 represents the Klein four-group symmetry. The first row corresponds to bosonic topological insulators and the second row to bosonic topological superconductors.

Symmetry	$d = 0$	$d = 1$	$d = 2$	$d = 3$
$U(1) \rtimes Z_2^T$	Z	Z_2	Z_2	Z_2^2
Z_2^T	Z_1	Z_2	Z_1	Z_2
$U(1)$	Z	Z_1	Z	Z_1
$SO(3)$	Z_1	Z_2	Z	Z_1
$SO(3) \times Z_2^T$	Z_1	Z_2^2	Z_2	Z_2^3
Z_n	Z_n	Z_1	Z_n	Z_1
$Z_2^T \times D_2 = D_{2h}$	Z_2^2	Z_2^4	Z_2^6	Z_2^9

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$$M^r(g)|g_0^r\rangle = v_2^{s(g)}(g_0^r, g^{-1}g^*, g^*)|gg_0^r\rangle, g^* = E$$

$$M^l(g)|g_0^l\rangle = v_2^{-s(g)}(g_0^l, g^{-1}g^*, g^*)|gg_0^l\rangle, g^* = E$$

$$(2)$$

where for $g \in Z_2^T$, $v_2(E, T, E) = v_2(T, E, T) = -1$, and $v_2(g_0, g_1, g_2) = 1$ otherwise. $s(g) = 1$ if g is unitary and $s(g) = -1$ if g is antiunitary. Here, $v_2(g^0, g^1, g^2)$ is the nontrivial 2-cocycle of Z_2^T , which is a function from three group elements to a $U(1)$ phase factor satisfying (21)

$$v_2^{s(g)}(g_0, g_1, g_2) = v_2(gg_0, gg_1, gg_2), g \in G$$

$$(3)$$

and

$$\frac{v_2(g_1, g_2, g_3)v_2(g_0, g_1, g_3)}{v_2(g_0, g_2, g_3)v_2(g_0, g_1, g_2)} = 1$$

$$(4)$$

For an arbitrary symmetry group G , if the ground-state wave function takes the dimer form as in Eq. 1 and symmetry acts on each right/left spin as in Eq. 2, then the edge spin forms a projective representation of symmetry G (labeled by v_2), and the state contains an SPT order protected by the symmetry (9, 12).

We can also use path integrals in (1+1)D to describe the 1D SPT phases, which allow us to generalize our result to higher dimensions. Because a 1D SPT phase is described by a cocycle v_2 , we can use the very same v_2 to construct the path integral for the SPT phase. To do so, we discretize the (1+1)D space time with a branched triangulation (Fig. 2A). For the Haldane chain, we associate a $g_i \in Z_2^T$ with each vertex of the space-time complex. Time reversal acts as complex conjugation K together with a mapping from g^i to

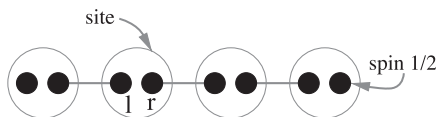


Fig. 1. Dimer form of the ground-state wave function in Haldane chain. Each site (big oval) contains two spin 1/2's (small dot), which are connected into singlet pairs (connected dots) between neighboring sites.

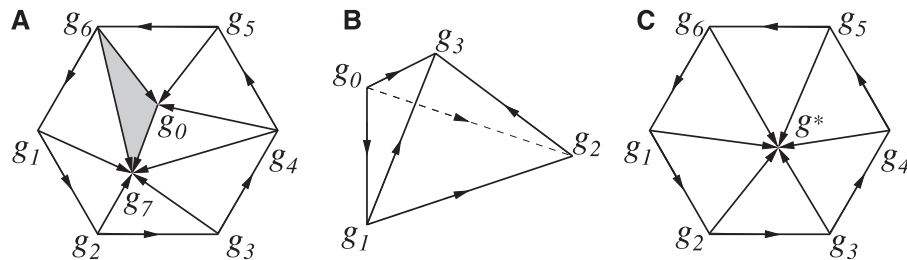


Fig. 2. (A) A branched triangulation of space time (21). Note that $s_{607} = -1$. (B) A tetrahedron, the simplest discrete closed surface. $\prod v^{s_{ijk}}(g_i, g_j, g_k) = 1$ on a tetrahedron is guaranteed by Eq. 4. Note that $s_{123} = s_{013} = 1$ and $s_{023} = s_{012} = -1$. (C) Discretized space-time manifold M_{ext} on an open disk with boundary manifold M . $g_j \in M$, g^* is in the interior of M_{ext} .

Tg^i . The path integral for the SPT phase then has the form

$$Z = |G|^{-N_v} \sum_{\{g_i\}} e^{-s(\{g_i\})},$$

$$e^{-s(\{g_i\})} = \prod_{\{ijk\}} v_2^{s_{ijk}}(g_i, g_j, g_k)$$

$$(5)$$

$|G|$ is the number of elements in G ($|G| = 2$ for Z_2^T), N_v is the number of vertices in the complex; $s_{ijk} = \pm 1$ depending on the orientation of the triangle. Because $v_2(Tg_0, Tg_1, Tg_2) = v_2^{-1}(g_0, g_1, g_2)$ (Eq. 3), the path integral is invariant under time reversal. (Similar construction works for any group.)

Because of Eq. 4, the path integral Eq. 5 actually describes a fixed-point theory, which does not change under coarse graining and retriangulation (21). For example, the path integral on the two triangulations (Fig. 2, A and C) is the same if we fix g_i 's on the boundary. Using this property, we can show that the action amplitude is always 1 on any orientable closed space-time surface, including the simplest discrete closed surface—a tetrahedron (Fig. 2B). So, g_i fluctuate strongly and the path integral describes a disordered phase that does not break the symmetry G .

To show that this path integral describes the SPT order in the Haldane chain, we need to calculate the ground-state wave function from the path integral that describes the imaginary time evolution from time $-\infty$ until time 0. In our formulation, this is equivalent to an imaginary time path integral on a space-time geometry with a boundary (at time 0). Denote the boundary as M and the whole manifold (a disk) as M_{ext} (Fig. 2A). As we are considering a fixed-point path integral, it does not matter how big the interior of M_{ext} is, and we can reduce it, for example, to just one point (Fig. 2C).

To obtain the ground-state wave function, we fix the degrees of freedom $\{g_i\}_M$ on M and find

$$\Psi(\{g_i\}_M) \propto \sum_{g^*} \prod_i v_2(g_i, g_{i+1}, g^*)$$

$$\propto \prod_i v_2(g_i, g_{i+1}, g^* = E),$$

$$(6)$$

where \prod_i is the product over all triangles on M_{ext} and, for simplicity of notation, we have chosen all triangles to be oriented clockwise.

The wave function on M does not depend on the choice of g^* . Time reversal acts as complex conjugation K together with a change of basis $|E\rangle \rightarrow |T\rangle$, $|T\rangle \rightarrow |E\rangle$ on each g_i , and the wave function is invariant under this action.

To show that the wave function Eq. 6 corresponds to the dimer state Eq. 1 (Fig. 1), we first expand each g_i into two degrees of freedom h_i^r and h_i^l such that $h_i^r = h_{i+1}^l = g_i$ (Fig. 3) and the amplitude of each configuration in the wave function remains unchanged, $\Psi(\{h_i^r = h_{i+1}^l = g_i\}) = \prod_i v_2(g_i, g_{i+1}, g^*)$. We then combine h_i^l and h_i^r into one site and apply a change of basis on each site

$$|h_i^l, h_i^r\rangle' = v_2(h_i^l, h_i^r, g^*)|h_i^l, h_i^r\rangle$$

$$= v_2(g_{i-1}, g_i, g^*)|h_i^l, h_i^r\rangle$$

The amplitude of all configurations in the new basis becomes 1, $\Psi(\{h_i^r = h_{i+1}^l = g_i\}) = 1$, which can be equivalently written as a product of dimers between neighboring sites $\Psi' = \prod_i \sum_{g_i} |h_i^r = g_i, h_{i+1}^l = g_i\rangle$. In this way, we have mapped each degree of freedom g_i into a dimer and the total wave function takes the same form as Eq. 1. Moreover, time-reversal symmetry acts on the edge degree of freedom as given by Eq. 2 (20). Therefore, our path integral Eq. 5 provides a proper description of the SPT order in the Haldane chain. To generalize this path-integral formulation to all spatial dimensions d and all symmetry groups G , we note that the two cocycles $v_2(g_0, g_1, g_2)$ used in the construction have higher dimensional analogs: the $(d+1)$ cocycles $v_{d+1}(g_0, \dots, g_{d+1})$, which are maps from $d+2$ group elements to a $U(1)$ phase factor and satisfy

$$v_{d+1}^{s(g)}(g_0, g_1, \dots, g_{d+1}) =$$

$$v_{d+1}(gg_0, gg_1, \dots, gg_{d+1}), g \in G$$

and

$$\prod_{i=0}^{d+2} v_{d+1}^{(-1)^i}(g_0, \dots, g_{i-1}, g_{i+1}, \dots, g_{d+2}) = 1$$

We use each $(d+1)$ cocycle v_{d+1} to construct a fixed-point path integral to describe an SPT state in d dimensions. The path integral is constructed by (i) discretizing the $(d+1)D$ space time with triangulation [triangle in (1+1)D, tetrahedron in (2+1)D, etc.]; (ii) assigning group element-labeled degrees of freedom to the vertices; and (iii) assigning action amplitude to each

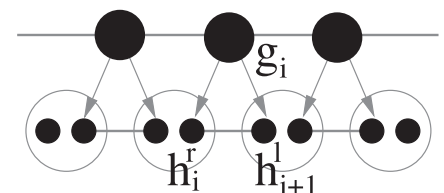


Fig. 3. Duality transformation between wave functions in Eq. 1 and Eq. 6.

simplex with the corresponding cocycle. The path integral then takes the form

$$z = |G|^{-N_v} \sum_{\{g_i\}} \prod_{\{ij...k\}} v_{d+1}^{s_{ij...k}}(g_i, g_j, \dots, g_k) \quad (7)$$

where $s_{ij...k} = \pm 1$ depends on the orientation of the simplex $ij...k$. Similar to the $(1+1)D$ case, it can be shown that the path integral is symmetric under symmetries in group G , and the action amplitude is in a fixed-point form and is quantized to 1 on a closed manifold (21). The ground-state wave function can be obtained from the action amplitude on an open geometry as discussed before $\Psi(\{g_i\}_M) = \prod_{\{i...j^*\}} v_{d+1}(g_i, \dots, g_j, g^*)$, where $\{g_i\}_M$ is on M and g^* is inside M_{ext} . $\prod_{\{i...j^*\}}$ is the product over all simplices. An exactly soluble Hamiltonian can be constructed to realize this state as the gapped ground state (21).

The nontrivial SPT order of the system can be seen explicitly from its boundary. The path integral of the degrees of freedom on the boundary can be obtained by putting the path integral on an open geometry as shown in Fig. 2C for $(1+1)D$. The manifold M now corresponds to the space-time manifold of the boundary degrees of freedom. The path integral for the boundary then reads

$$Z_b = |G|^{-N_v} \sum_{\{g_i\}} \prod_{\{i...j^*\}} v_{d+1}^{s_{i...j^*}}(g_i, \dots, g_j, g^*) \quad (8)$$

which only depends on $\{g_i\}_M$ on the boundary M and does not depend on g^* , which is inside M_{ext} .

This term can be thought of as a discretized version of the Wess-Zumino-Witten (WZW) term (22, 23) in nonlinear σ models because (i) it is a path integral of $(d-1)+1$ dimensional systems written on an extended $(d+1)D$ manifold with a boundary; (ii) the action amplitude does not depend on how the extended field in the interior of the $(d+1)D$ manifold is chosen; and (iii) its field takes value in a group G , and the path integral is invariant under the action of $g \in G$. On the other hand, this term is more general than the original continuous WZW term because it applies to discrete groups like Z_2^T while the continuous WZW term only works for continuous groups. We expect that the boundary states described by such a discretized WZW term will be gapless/degenerate as long as symmetry is not broken, similar to systems described by continuous WZW terms. This has been firmly established in $(1+1)D$ and $(2+1)D$. In $(1+1)D$, as with the example of Haldane chain, symmetry action on the edge degree of freedom does not have a 1D representation; therefore, the edge state will always be degenerate. In $(2+1)D$, it has been proven using the tool of matrix product unitary operator that the boundary must be gapless as long as symmetry is not broken (24, 25). Therefore, the boundary of the systems we constructed carries gapless/degenerate states protected by certain symmetry, which reflects the nontrivial SPT order of the system.

The numbers of nontrivial SPT phases constructed using cocycles for some simple symmetry groups are summarized in Table 1. We find one kind of bosonic topological insulator in 2D and three kinds in 3D with boson number-conservation symmetry $U(1)$ and time-reversal symmetry Z_2^T . If boson numbers are not conserved but time-reversal symmetry Z_2^T is preserved, then we find one kind of bosonic topological superconductor in every odd spatial dimension. Our construction is nonperturbative and works for strongly interacting bosonic systems. Therefore, it contributes to a more complete understanding of the topological phase diagram in strongly correlated quantum systems.

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Supplementary Materials

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Sign-Problem-Free Quantum Monte Carlo of the Onset of Antiferromagnetism in Metals

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The quantum theory of antiferromagnetism in metals is necessary for our understanding of numerous intermetallic compounds of widespread interest. In these systems, a quantum critical point emerges as external parameters (such as chemical doping) are varied. Because of the strong coupling nature of this critical point and the “sign problem” plaguing numerical quantum Monte Carlo (QMC) methods, its theoretical understanding is still incomplete. Here, we show that the universal low-energy theory for the onset of antiferromagnetism in a metal can be realized in lattice models, which are free from the sign problem and hence can be simulated efficiently with QMC. Our simulations show Fermi surface reconstruction and unconventional spin-singlet superconductivity across the critical point.

The presence of an antiferromagnetic transition in a metal is common to compounds such as electron-doped cuprates (1), iron-

based superconductors (2), and heavy fermion Kondo lattice systems (3). Whereas our understanding of quantum antiferromagnetism in insulators has seen major advances (4), analogous problems in metals are far more complicated because of the subtle interplay between the low-energy fermionic quasiparticles on the Fermi surface, and the quantum fluctuations of the antiferromagnetic order parameter. In addition, the presence of the Fermi surface has hampered large-scale numerical studies, because quantum Monte Carlo (QMC) algorithms are afflicted by the well-known fermion

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